Indian J. Phys. **52B**, 58–61 (1978)

Thermal conductivity of oxygen

P. C. JAIN

National Physical Laboratory, New Delhi-110012

AND

T. P. PANDYA

Lucknow University, Lucknow, U.P.

(*Received* 6 *April* 1977, *revised* 6 *August* 1977)

The values of thermal conductivity of oxygen computed from kinetic theory expression in conjunction with the recently proposed $STPO_2I$ potential and the three theoretical expressions for f have been compared with the experimental data generated by Jain and Saxena. The vibrational energy diffusion coefficients have also been computed as a function of temperature.

1. INTRODUCTION

The recent thermal conductivity data for oxygen (accuracy about 2%) due to Jain and Saxena (1977) have been used for evaluating the suitability of theoretical expressions proposed for predicting the thermal conductivity (k) of gases and also for calculating the vibrational energy diffusion coefficients of the gas.

2. THEORETICAL EXPRESSIONS

The thermal conductivity of gases can be calculated with the help of the kinetic theory expression (Hirschfelder *et al* 1967), corrected in the case of a polyatomic gas, for the transport of energy by internal modes. The three Eucken type correction factors, f, suggested by Hirschfelder (1957), Mason and Monchick (1962) and Saxena *et al* (1964) are respectively as follows :

$$f(H) = 0.115 + 0.354(C_p/R) \qquad \ldots (1)$$

$$f(M) = \frac{4}{15R}\,(f_{tr}C_{v,tr} + f_{int}\,C_{v,int}) \qquad \ldots (2)$$

$$f(S) = f(H) - \left(\frac{5}{2} - \frac{\rho D_{int}}{\mu}\right)\left(\frac{C_{v,int}}{C_v Z}\right) \qquad \ldots (3)$$

Here C_p is the specific heat at constant pressure, R is the gas constant, f_{tr} and f_{int} are respectively the translational and internal contributions to f, $C_{v,tr}$ and $C_{v,int}$ are the translational and internal contributions to the total specific heat at constant volume, C_v, ρ is the density, μ is the viscosity, D_{int} is the internal energy diffusion coefficient and Z is the number of molecular collisions required to exchange a quantum of internal energy with translational energy.

The calculation of k involves the use of a suitable intermolecular potential. The Thakkar and Smith (1975) potential ($STPO_2I$) has shown a good agreement with the experimental values of a number of physical properties of oxygen. Its parameters ($\epsilon/k_B = 130.8K$ and $\sigma = 3.326$Å) have been, therefore, used in the present calculations by making the following substitutions :

$$D_{int} \quad D \text{ and } \frac{\rho D}{\mu} = \frac{6}{5} A^*$$

where D is the self diffusion coefficient, A^* is the ratio of the collision integrals and is in turn, a function of the reduced temperature, T^*.

For oxygen :

$$C_{v,rot} = R, \quad C_{v,tr} = 3/2(R) \text{ and } C_{v,int} = C_p - 2.5R$$

and the estimates of C_p values are given by Svehla (1962). The value of Z has been given by Annis and Malinauskas (1971) as 5.6 at 475K. Using the limiting value of Z at high temperature, Z^∞, as 22.8 in Parker's (1959) expression (with the correction introduced by Brau and Jonkman (1970), the values of Z as a function of temperature are generated for use in Eq. (3).

3. Comparison with Experimental Data

The computed values of thermal conductivity are compared with the experimental data in figure 1. A comparison of the data with those computed from the expression due to Keyes (1951) is also given in the same figure.

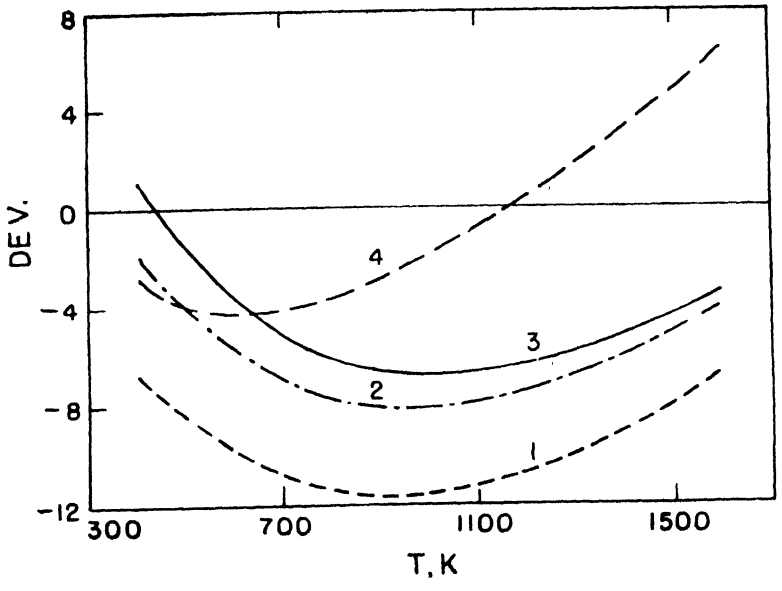

Fig. 1. Comparison of experimental k data with theoretical values. Curves 1-4 are based on the theories of Hirschfelder (1957), Mason and Monchick (1962), Saxena *et al.* (1964) and Keyes (1951) respectively.

4. Discussion

The agreement between theory and experiment is not quite satisfactory in any case. The values based on the macroscopic theory of Saxena *et al* (1964) are, however, the best of all, the average absolute and maximum deviations being 4.7 and 6.7 percent respectively. The deviations in all the three cases are practically the same as those found by Jain and Saxena (1977) using the m-6-8 potential, which shows that the m-6-8 and S-T potentials lead to the same results. Keyes correlation is valid for the temperature range 90-375K. In the temperature range 400-1600K, the average absolute and maximum deviations between experimental data and Keyes correlation are 3.2 and 6.2 percent respectively. This agreement is much better than in the cases of the other three theoretical expressions over the entire temperature range.

5. Vibrational Energy Diffusion Coefficient

Following Ahtye (1972), the D_{vib}/D values have been computed by using the ρ values (Hilsenrath *et al* 1955) and the parameters of the $STPO_2I$ potential. The results are given in table 1. A comparison with those due to Jain and Saxena shows a deviation as high as 41.4% at 700K, but this deviation is found to decrease rapidly with increasing temperature.

Table 1. D_{vib}/D as a function of temperature

T, K	D_{vib}/D	
	Present work	Jain & Saxena (1977)
700	0.29	0.41
800	0.34	0.43
900	0.38	0.45
1000	0.43	0.48
1100	0.47	0.51
1200	0.51	0.54
1300	0.57	0.58
1400	0.62	0.62
1500	0.68	0.67
1600	0.73	0.72

References

Ahtye W. F. 1972 *J. Chem. Phys.* **57**, 5542.
Annis B. K. & Malinauskas A. P. 1971 *J. Chem. Phys.* **54**, 4763.
Brau C. A. & Jonkmann R. M. 1970 *J. Chem Phys.* **52**, 477.

Hilsenrath J., Beckett C. W., Benedict W. S., Fano L., Hoge H. J., Masi J. F., Muttall R.L., Touloukian Y. S. & Woolley H. W. 1955 *Tables of Thermal Properties of Gases,NBS Circular No.* 564.

Hirschfelder J. O. 1957 *J. Chem. Phys.* **26**, 282.

Hirschfelder J. O., Curtiss C. F. & Bird R. B. 1967 *Molecular Theory of Gases and Liquids* (Wiley, New York) 534-540.

Jain P. C. & Saxena S. C. 1977 *Molecular Phys.* **33**, 133.

Keyes F. G. 1951 *Trans. ASME* **73**, 589.

Mason E. A. & Monchick L. 1961 *J. Chem. Phys.* **56**, 1622.

Parker J. C. 1959 *Phys. Fluids* **2**, 449.

Saxena S. C., Saksena M. P. & Gambhir R. S. 1964 *Brit. J. Appl. Phys.* **15**, 843.

Svohla R. A. 1962 *Estimated Viscosities and Thermal Conductivities of Gases*, NASA Tech. Report TR-R 132, 98.

Thakkar A. J. & Smith V. H. 1975 *Mol. Phys.* 29, 731.